A spatial interpretation of emerging superconductivity in lightly doped cuprates

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The formation of domains comprising alternating hole rich and hole poor ladders recently observed by Scanning Tunneling Microscopy by Kohsaka et al., on lightly hole doped cuprates, is interpreted in terms of an attractive mechanism which favors the presence of doped holes on Cu sites located each on one side of an oxygen atom. This mechanism leads to a geometrical pattern of alternating hole-rich and hole-poor ladders with a periodicity equal to 4 times the lattice spacing in the CuO plane, as observed experimentally. To cite this article: G. Deutscher, P.-G. de Gennes, C. R. Physique 8 (2007).

I. INTRODUCTION

Recent imaging of Scanning Tunneling Spectroscopy (STM) of lightly doped superconducting cuprates has revealed the existence of rectangular domains of width 4a, where a is the lattice spacing in the CuO plane [1]. Inside each domain the carrier concentration is non-uniform, with a sharp contrast between a central ladder consisting of a column of oxygen atoms and the two neighboring Cu-O-Cu columns where the carrier concentration is high, while it is low on similar ladders at the edges of the domain. The general aspect of the images shows domains having two possible orientations at right angles to each other, with less well organized domains spread randomly across the surface. Tunneling characteristics measured at sites belonging to the central ladder show at low bias a structure reminiscent of a superconducting density of states, with pronounced peaks particularly on the Cu-O-Cu columns, while at the edge ladders only a small conductance dip is visible.

In this communication we wish to point out that this geometrical pattern can be easily understood if one assumes the existence of a mechanism that favors the presence of a pair of doped holes on Cu-O-Cu, or perhaps O-Cu-O-Cu-O segments, accompanied by a small contraction of the Cu-O distances. This mechanism can be due to an increase of the transfer integral t_{OCu}. t_{OCu} depends critically on the overlap between Cu(d) orbitals and O(p) orbitals. If the energy gained by contraction is sufficient, a bound state of the hole pair can be formed.

II. THE MODEL

Our interpretation of the pattern observed in [1] proceeds in three steps: (i) Pair formation; (ii) Formation of holerich and hole-poor regions; (iii) Pair propagation.

A. Pair formation

We discuss on Fig. 1 the binding energy of a hole pair on a Cu-O-Cu segment. We estimate it by a variational function containing four states α, β, γ' and γ'' as defined in Fig. 1(b). We are interested here in the spin singlet, for which the amplitudes are even ($\alpha = \beta, \gamma' = \gamma''$). The unperturbed energy of (α) and (β) is U and is large. The eigenvalue equation for the energy ϵ is then:

$$\epsilon(\epsilon - U) = 4(t_{OCu})^2 \tag{1}$$

This leads (for large U) to an energy:

$$\epsilon_{pair} = -4(t_{OCu})^2/U \tag{2}$$

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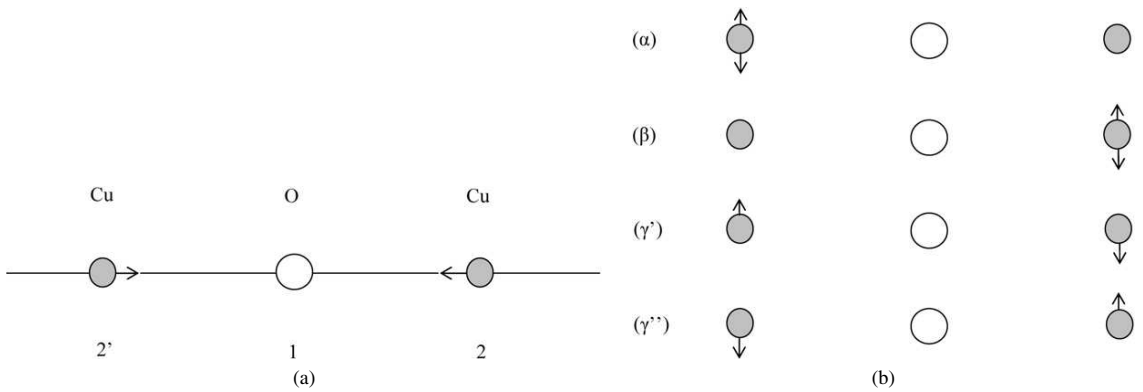

FIG. 1: (a) A two hole pair on two copper atoms (2) and (2'), around one oxygen atom (1). We assume here that the two coppers move in when each of them carries a hole: the transfer integral between 2 and 2' is increased. (b) The four states participating in the construction of a spin singlet pair.

FIG. 2: (a) An oxygen centered O-Cu-O-Cu-O segment with holes located on the edge oxygens. Energy is lowered by admixture with states as shown in Fig. 2b.

(We are indebted to W. Harrison for pointing out the factor 4 showing up in the singlet energy.) We must compare this to the energy of two independent holes, both at the bottom of the band, $2\epsilon_0$, where $\epsilon_0 = 4t_0$ is the half band width. The pairs win if:

$$t_{OCu} = (Ut_0/2)^{1/2} \tag{3}$$

On the whole, this idea is very tentative but it has one merit: the ratio t_{Ocu}/t_0 is very sensitive to the (Cud)(O p) overlap; this could explain why ions which are isoelectronic to Cu cannot compete with the cuprates.

There is, however, a difficulty with holes residing on copper atoms, in view of the high ionization potential of the Cu^{++} ion [2]. Holes may reside preferentially on oxygen atoms. This can be achieved if we consider a O-Cu-O-Cu-O segment, with holes on the edge oxygen atoms (Fig. 2). Here, energy can be gained by admixture with states where a hole is transferred from one of the coppers to the central oxygen. The energy gained is still proportional to $(t_{OCu})^2$.

B. Formation of hole-rich and hole-poor regions

So let us assume that two holes have formed a bound state, and let us examine the consequences for the neighboring sites, as shown in Fig. 3. Following Kohsaka et al. we label 1 the site of the central oxygen atom; 2 and 2' the neighboring copper sites; 3 and 3' the following copper sites, followed by the oxygen sites 4 and 4'. Since the contraction, or dimerisation, of the segment (2-2') goes hand in hand with a local increase of the hole density, it follows that the hole density on neighboring sites such as copper sites 3 and 3' is decreased. A charge density wave can be triggered by local pair formation, dimerisation and the charge density wave being coupled phenomena, the two reinforcing each other. We then arrive at the following sequence: the central Cu-O-Cu bond (2'-1-2) is hole-rich, the neighboring bonds (3-4) and (4'-3') are hole-poor. Over a distance of 4a, there are two hole-rich and two hole-poor Cu sites. Defects, due primarily to independent nucleation of other dimers at right angles with the one under consideration, will pin the charge density wave. The pair on 2'-2 cannot propagate along its axis. These conclusions still hold if the hole pair is localized on a five site segment.

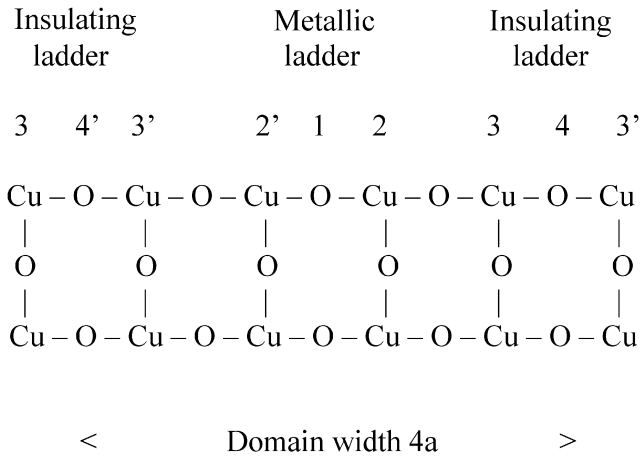

FIG. 3: The pattern of hole concentration in a domain consisting of one high concentration central ladder centered on a column of oxygen atoms with two low concentrations ladders on each side. The pattern leads to a periodicity of 4 times the lattice parameter of the CuO plane.

C. Pair propagation

There is nothing to prevent pair propagation in the perpendicular direction, which will reduce the kinetic energy. This will lead to the formation of domains consisting of one central hole-rich and two lateral hole-poor ladders, the central ladder being centered on an oxygen column. Pair propagation on the central ladder can lead to incipient superconductivity. A periodicity of 4a (1), as has been observed, with alternating conducting (and may be superconducting), and insulating (and may be antiferromagnetic) domains can be favorable in some range of doping, see below a discussion of this point.

Domain formation is the result of a nucleation process of the first bound state. This nucleation process occurs randomly along the (10) and (01) directions, resulting in domains at right angles randomly distributed, again as observed. There is no long range order in this pattern.

III. DISCUSSION

The essential difference between the proposed model and that of stripes [3, 4, 5] is that ours is not a purely electronic one reflecting the competition between AF and superconducting orders, where the lattice plays no role (or only a very secondary one). Rather, the contraction of Cu-O bonds plays here a central role. Both models predict oxygen centered structures, in agreement with experiments [1, 6], but differ in some important ways. While stripes are basically one dimensional (namely their length should be much longer than their width), our model being based on a local bond contraction leads to a pattern of domains, at right angles to each other, that are not necessarily very long, in better agreement with what is observed [1], and with several pieces of experimental evidence for an Electronic Cluster Glass in underdoped samples ([7] and references therein), rather than one dimensional stripes. Lattice disorder below the temperature of formation of the domains is a natural consequence of our local pair formation model, since bond contraction is local and occurs randomly in two different directions. Lattice disorder has indeed been found to increase below a temperature of about 150 K, which we surmise is that of formation of the domains [8, 9].

The hole doping level of the samples studied by Kohsaka et al. is of the order of 0.1 per Cu site. The minimum number of Cu sites necessary to have at least one hole pair per domain is then 20, which means that slightly elongated domains as observed do contain a few hole pairs. Conduction can take place along the central ladder. If we assume that the hole concentration is peaked on the central ladder and is negligible on the edge ladders, the hole concentration on the central ladder is then of the same order as the average concentration at optimum doping. The edge ladders are then at a concentration near that of the pure antiferromagnetic phase. Barring complications due to the one-dimensional character of the central ladders, one may also expect the formation of a superconducting gap of the same order of magnitude as that of the gap at optimum doping, i.e. of a few 10 meV, again as observed.

The emerging picture of a lightly doped cuprate is then that it is composed of conducting and superconducting ladders weakly coupled together, either laterally through insulating ladders or at right angles. Conduction and

superconduction on the macroscopic scale will necessarily require coupling between ladders oriented at right angles. Since translational and rotational symmetry are broken in the ladder pattern, which is highly disordered, it is not obvious that quasi-particles can exist with a well defined wave vector formed in lightly doped cuprates. Indeed, the normal state is known to be weakly insulating. If some degree of coherence can be achieved, one may expect that it will be for quasi-particles having their momentum at 45 degrees from the ladders directions, which is the (11) orientation and equivalent. Clearly, there is no possibility of propagation along the (10) and equivalent directions because of the interruption of the domains. This is in agreement with the known fact that lightly doped cuprates have an incomplete Fermi surface consisting of small arcs around the (11) directions [10].We note that strong renormalization effects near the Fermi level around the (11) direction over an energy range of the order of 100 meV have recently been attributed to electronphonon interaction [11].

Superconductivity on themacroscopic scale can be very different from that in the individual domains, again because it requires coupling between domains that are at right angles from each other. A gap anisotropy is to be expected, with the strongest gap values being along the (10) and equivalent directions. It may be that this coupling is also at the origin of the d-wave symmetry of the macroscopic superconducting order parameter.

Note added by Guy Deutscher at the time of submission of the final version Pierre-Gilles de Gennes passed away a few days before we were to have a final discussion of the manuscript. He had left clear instructions that I was to take care of the final version. It is under these very sad circumstances that this revised version is being submitted. Had we met as planned, the final version might of course have been somewhat different but in view of the intense correspondence that we had in the period of several weeks preceding his death, I feel reasonably sure that this version is close to what he wanted it to be. In any case, I have done the best I could. Warm thanks are due to Philippe Nozires for a critical reading of the manuscript.

Acknowledgments

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